Multipole expansion of Bessel and Gaussian beams for Mie scattering calculations

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Multipole expansions of Bessel and Gaussian beams, suitable for use in Mie scattering calculations, are derived. These results allow Mie scattering calculations to be carried out considerably faster than existing methods, something that is of particular interest for time evolution simulations where large numbers of scattering calculations must be performed. An analytic result is derived for the Bessel beam that improves on a previously published expression requiring the evaluation of an integral. An analogous expression containing a single integral, similar to existing results quoted, but not derived, in literature, is derived for a Gaussian beam, valid from the paraxial limit all the way to arbitrarily high numerical apertures. © 2009 Optical Society of America

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1. INTRODUCTION

Generalized Lorenz–Mie theory (GLMT) is a powerful tool for theoretical and numerical investigation of optical trapping phenomena [1–3]. The computationally demanding steps are solving for the field in the case of multiple scattering between several nearby particles, the calculation of the force on a particle, and the calculation of the beam shape coefficients (BSCs). Several different approaches exist for efficiently handling multiple scattering [4,5], and series expressions for the force on a particle have been published [6]. If these techniques are implemented effectively, the speed of the calculation can be limited by the time required to calculate the BSCs, which represent the electromagnetic field in the form of a multipole expansion. Hence there is a need for efficient ways to calculate the beam shape coefficients for a given beam type. This is particularly important for time evolution simulations where large numbers of scattering calculations must be performed [7–9]

The BSCs can be determined for an arbitrary field $\mathbf{E}(\mathbf{r})$ by exploiting the orthogonality of the vector spherical harmonics and performing an eigenfunction transform, as outlined below in Eq. (2). However this approach is slow as it requires the evaluation of a surface integral. Alternative approaches involving systems of linear equations [10] are fairly efficient at the focus of a tightly focused beam, but are not suited to arbitrary positions or lower numerical apertures (NAs). Fast approximate methods exist that can be applied to particles whose radius is smaller than the beam waist (the localized approximation [11]) or for particles very close to the beam waist [12], but there is often a need for a solution that does not fit these constraints (see, for example, [13]).

For a plane wave Eq. (2) can be solved analytically to determine the beam shape coefficients [1], but the calculation is more difficult for beams commonly used in optical trapping and manipulation experiments. Here we present a full analytic solution to the BSCs for a Bessel beam through consideration of its plane wave spectrum. This contrasts with existing published results that require the evaluation of a surface integral [8]. We also show how a similar approach can be applied to a fully vectorial Gaussian beam to obtain results similar to those published by Maia Neto and Nussenzveig [14] and Mazolli *et al.* [15]. Finally we compare the time required for the different approaches.

GLMT exploits the symmetry of a spherical particle and expresses the electric field $\mathbf{E}(\mathbf{r})$ of the beam in terms of the vector spherical harmonics $\mathbf{M}^{(1)}_{mn}$ and $\mathbf{N}^{(1)}_{mn}$ [1]. Here we use the expansion

$$\mathbf{E} = -i\sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}(p_{mn}\mathbf{N}^{(1)}_{mn} + q_{mn}\mathbf{M}^{(1)}_{mn}). \tag{1}$$

Since the vector spherical harmonics form a complete orthogonal set we can recover the BSCs p_{mn} and q_{mn} through an eigenfunction transform,

$$p_{mn} = i\sqrt{\frac{4\pi}{2n+1}\frac{(n+m)!}{(n-m)!}} \times \frac{\int_0^{2\pi}\int_0^{\pi}\mathbf{E}\cdot\mathbf{N}^{*}_{mn}\sin\theta \mathrm{d}\theta \mathrm{d}\phi}{\int_0^{2\pi}\int_0^{\pi}|\mathbf{N}_{mn}|^2\sin\theta \mathrm{d}\theta \mathrm{d}\phi}, \tag{2}$$

and similarly for q_{mn}, using $\mathbf{M}_{mn}$ instead of $\mathbf{N}_{mn}$.

It is worth noting at this point that a number of different conventions exist for the exact form of the beam expansion. Barton *et al.* [6] and Čižmár *et al.* [8] use a slightly different version of Eq. (1). If ka is the size parameter of the sphere and n_{ext} is the refractive index of the external medium, then their BSCs A_{lm} and B_{lm} are related to our p_{mn} and q_{mn},

$$A_{lm} = \frac{ip_{mn}}{2\pi(ka)}, \quad B_{lm} = \frac{n_{ext}q_{mn}}{2\pi(ka)}. \tag{3}$$

2. BESSEL BEAM EXPANSION

The nondiffracting properties of Bessel beams make them of interest for optical confinement experiments. Čižmár *et al.* [8] derived a method of calculating BSCs for a Bessel beam that required the evaluation of a single integral for each coefficient. Here we derive an analytic result that does not require the numerical evaluation of any integrals and hence is considerably faster to compute.

Consider a sphere at position $\mathbf{r}_0=(x,y,z)$, which is exposed to the field of an x-polarized Bessel beam propagating along the z axis. We represent the beam by a sum of plane waves $\mathbf{e}_0 e^{i\mathbf{k}\cdot\mathbf{r}}$ making an angle θ with the z axis [8],

$$\mathbf{E}(\mathbf{r}) = E_0 \int_0^{2\pi} \mathbf{e}_0(\theta,\phi) e^{i\mathbf{k}\cdot\mathbf{r}} \mathrm{d}\phi, \tag{4}$$

where $\mathbf{k}=(k,\theta,\phi)$ (in polar coordinates) and $\mathbf{e}_0=\cos\phi \mathbf{i}_\theta - \sin\phi \mathbf{i}_\phi$.

The coefficients p_{mn} and q_{mn} for a plane wave $\mathbf{e}_0 e^{i\mathbf{k}\cdot\mathbf{r}}$ expanded about the sphere at $\mathbf{r}_0$, in terms of the modified Legendre polynomial P_n^m, are [16], Eq. (20)

$$\begin{Bmatrix} p_{mn} \\ q_{mn} \end{Bmatrix} = U_n \left(\mathbf{e}_\theta \begin{Bmatrix} \tilde{\tau}_{mn} \\ \tilde{\pi}_{mn} \end{Bmatrix} - i\mathbf{e}_\phi \begin{Bmatrix} \tilde{\pi}_{mn} \\ \tilde{\tau}_{mn} \end{Bmatrix} \right) e^{-im\phi} e^{i\mathbf{k}\cdot\mathbf{r}_0},$$

$$U_n = \frac{4\pi i^n}{n(n+1)},$$

$$\tilde{\pi}_{mn}(\cos\theta) = \sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}} \frac{m}{\sin\theta} P_n^m(\cos\theta),$$

$$\tilde{\tau}_{mn}(\cos\theta) = \sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}} \frac{d}{d\theta} P_n^m(\cos\theta). \tag{5}$$

We substitute the plane wave expansion in Eq. (5) into Eq. (4), giving

$$\begin{Bmatrix} p_{mn} \\ q_{mn} \end{Bmatrix} = E_0 U_n \times \int_0^{2\pi} \left[\cos(\phi) \begin{Bmatrix} \tilde{\tau}_{mn} \\ \tilde{\pi}_{mn} \end{Bmatrix} + i\sin(\phi) \begin{Bmatrix} \tilde{\pi}_{mn} \\ \tilde{\tau}_{mn} \end{Bmatrix} \right] e^{-im\phi} e^{i\mathbf{k}\cdot\mathbf{r}_0} \mathrm{d}\phi. \tag{6}$$

The $e^{i\mathbf{k}\cdot\mathbf{r}_0}$ term can be expanded, and sine and cosine rewritten in terms of exponentials, for $\rho=k\sqrt{x^2+y^2}\sin\theta$ and $\phi_0=\arctan(-y/x)-(\pi/2)$ to obtain

$$\begin{Bmatrix} p_{mn} \\ q_{mn} \end{Bmatrix} = E_0 U_n e^{ikz\cos\theta} \times \left[\begin{Bmatrix} \tilde{\tau}_{mn} \\ \tilde{\pi}_{mn} \end{Bmatrix} I^+ + \begin{Bmatrix} \tilde{\pi}_{mn} \\ \tilde{\tau}_{mn} \end{Bmatrix} I^- \right],$$

$$I^\pm = \frac{1}{2}\int_0^{2\pi} e^{i(1-m)\phi} e^{i\rho\cos[\phi+\phi_0+(\pi/2)]} \mathrm{d}\phi \pm \frac{1}{2}\int_0^{2\pi} e^{i(-1-m)\phi} e^{i\rho\cos[\phi+\phi_0+(\pi/2)]} \mathrm{d}\phi. \tag{7}$$

Using result 9.1.21 from [17] the azimuthal integral can be solved in terms of Bessel functions of the first kind to give

$$I^\pm = \pi(e^{i(m-1)\phi_0} J_{1-m}(\rho) \pm e^{i(m+1)\phi_0} J_{-1-m}(\rho)). \tag{8}$$

The field described by Eqs. (1) and (7) has been verified to be the same as the explicit integral in Eq. (4). With the integral eliminated, the BSCs can be calculated analytically in a fraction of the time required by existing published methods.

3. FULLY VECTORIAL GAUSSIAN BEAM EXPANSION

Representing a tightly focused Gaussian beam presents challenges, and much effort has been devoted to increasingly detailed nth order approximation to the beam [18–20]. Such a perturbative approach cannot be applied to optical tweezers, where the NA can be greater than 1. It is, however, possible to accurately describe the far-field of a tightly focused Gaussian beam, and Nieminen *et al.* exploit this to build a system of linear equations that can be solved to obtain the BSCs [10]. We refer to [10] for a discussion of some of the issues relating to multipole expansion of tightly focused beams.

It is also possible to derive a single integral expression for the BSCs from the far-field expansion, and results have been published for a circularly polarized Gaussian beam (without details of the derivation) by Maia Neta and Nussenzveig [14] and Mazolli *et al.* [15]. Here we derive analogous results for a linearly polarized Gaussian beam and compare the performance of this method with the approach of Nieminen *et al.* [10]. Ours is a universal expansion that can be applied to any Gaussian beam from the plane wave limit through to high NA beams.

We exploit the orthogonality of the vector spherical harmonics to solve the surface integral of Eq. (2). For mathematical convenience, we elect to evaluate the p_{mn} surface integral at radius $kR=[2N\pi+(n\pi/2)]$ and the q_{mn} surface integral at radius $kR=\{2N\pi+[(n+1)\pi/2]\}$, in the limit of large N. Under these conditions, the vector spherical harmonics are

$$\sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}} \begin{Bmatrix} \mathbf{N}_{mn} \\ \mathbf{M}_{mn} \end{Bmatrix} = \left(\begin{Bmatrix} \tilde{\tau}_{mn} \\ i\tilde{\pi}_{mn} \end{Bmatrix} \mathbf{i}_\theta + \begin{Bmatrix} i\tilde{\pi}_{mn} \\ -\tilde{\tau}_{mn} \end{Bmatrix} \mathbf{i}_\phi \right) \frac{e^{im\phi}}{kR}. \tag{9}$$

We represent a fully vectorial Gaussian beam in the far field by [21],

$$\mathbf{E} = \frac{E_0 k^2 w_0^2}{2ikR} \sqrt{\cos\theta} e^{-(\gamma\sin\theta)^2} e^{ikR} e^{i\mathbf{r}\cdot\mathbf{i}_r} (\cos\phi \mathbf{i}_\theta - \sin\phi \mathbf{i}_\phi), \tag{10}$$

where γ is the ratio of the focal length of the objective to the beam waist size of the (broad) Gaussian beam *before* the objective. We have selected the global amplitude and phase to be consistent with the plane wave result in Eq. (5).

Substituting these into Eq. (2), and expressing the azimuthal integral as before in terms of $I^{\pm}$, which we solved in Eq. (8), we find

$$\begin{Bmatrix} p_{mn} \\ q_{mn} \end{Bmatrix} = U_n \int_0^{\theta_0} E'(\theta) \left(\begin{Bmatrix} \tilde{\tau}_{mn} \\ \tilde{\pi}_{mn} \end{Bmatrix} I^+ + \begin{Bmatrix} \tilde{\pi}_{mn} \\ \tilde{\tau}_{mn} \end{Bmatrix} I^- \right) \sin\theta \mathrm{d}\theta, \tag{11}$$

where $E'(\theta) = (E_0 k^2 w_0^2 / 4\pi) \sqrt{\cos\theta} e^{-(\gamma \sin\theta)^2} e^{ikz\cos\theta}$ and θ_0 is the half-angle subtended by the objective at the beam focus.

It can be seen that this result is analogous to Doicu and Wriedt's Eq. (21) [18], which holds in the limit of low NA, but the result here is valid for tightly focused beams as well. Our result is also consistent with that quoted but not derived by Mazolli *et al.* for a circularly polarized beam [15]. Finally we note that since the θ integral cannot be solved analytically, the envelope $E'(\theta)$ can be modified as required, and hence it is trivial to impose radially symmetric modifications to the beam profile, such as apodization.

4. PERFORMANCE COMPARISON

We compared the performance of our formulas to the existing algorithms for calculating the BSCs. The details of the coefficients and methods compared are as follows:

- Sphere size parameter $ka = 19$, selected as characteristic of particles in our experiments. This leads to the requirement that $n_{\max} = 32$ [1,22] for low-NA beams, but $n_{\max}$ can take smaller values close to a high-NA focus, as discussed in [10].
- Convergence condition on the calculated force was a relative error below 10^{-3}. There is absolutely no need for higher accuracy when comparing with experiments, since there is liable to be considerably more uncertainty than that on some of the experimental parameters.
- The execution time was measured for single-threaded *C* code running on an Intel Core 2 Duo processor. Single-threaded performance is reported since in general any threading of the code should be done at a higher granularity than a single BSC calculation.
- For broad Gaussian beams, and the Bessel beam, the BSCs for an off-axis sphere were calculated directly from the relevant integrals. For these broad-waisted beams the translation addition theorem is *not* used as described in [10] as the advantage of it is lost when the beam waist size is significantly larger than the particle radius: a prohibitively large $n_{\max}$ is required.
- For high-NA Gaussian beams we only report timings for a particle at the beam focus, in recognition of the fact that the most efficient way of determining the expansion at other locations is to use the translation addition theorem to transform the expansion at the beam focus [10].
- Numerical integrations were performed using Simpson's rule. For the specified convergence level, we typically found that the integrand was being evaluated a few tens of times.
- In the on-axis case the rotational symmetry of the beam was exploited to reduce the number of coefficients requiring evaluation.
- In the two-sphere multiple scattering calculation shown for comparison in Fig. 1, translation between spheres made use of the recurrences and translation–rotation decomposition techniques described in [4].
- When solving a linear system of equations (using far-field fitting) to obtain the timings shown in Fig. 2, the rotational symmetry of the beam was exploited and no over-determination was present in the system of equations (in order to obtain the fastest possible speed for comparison with our method).
- The least-squares matrix calculation was performed with the help of a commercial basic linear algebra subprogram (BLAS) package provided by Apple Computer Inc., and all other performance-critical calculations were performed using hand-optimized custom *C* code.
- Approximate methods such as the generalized minimal residual (GMRES) algorithm might offer a faster alternative way to carry out BSC calculation of Nieminen *et al.* [10]. We investigated this briefly but found that although this might in principle be faster, it was unusually sensitive to what initial guess was provided for the BSCs and so we did not pursue this avenue any further.

The speed of the BSC calculation is the limiting factor in a single-sphere calculation when it takes longer than

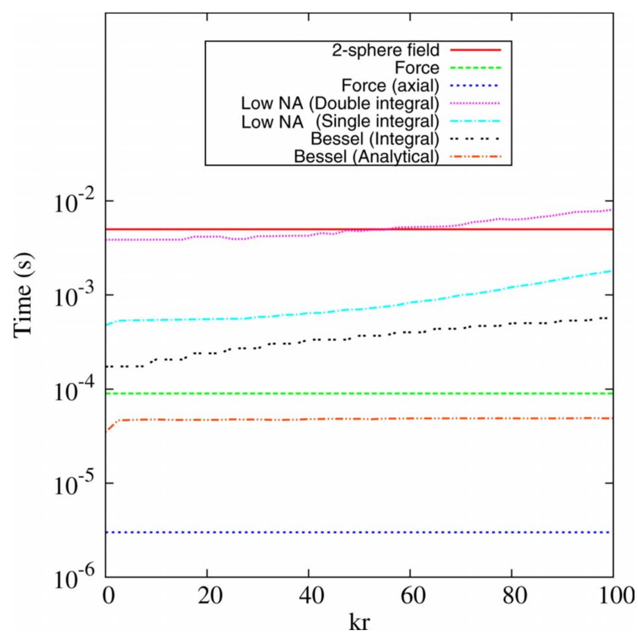

Fig. 1. (Color online) Execution time for alternative BSC calculation algorithms as a function of sphere radial position kr relative to the beam axis. For low NAs our single integral calculation is shown to be roughly ten times faster than a double integral calculation over the plane wave decomposition of the beam. For a Bessel beam our analytical result is shown to be up to ten times faster than a single integral calculation. For reference, execution times are also shown for force calculation and for a two-sphere multiple scattering calculation.

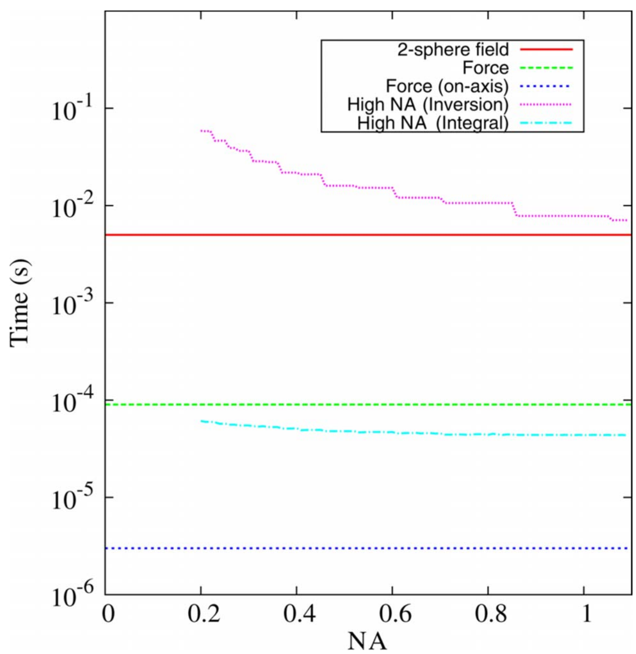

Fig. 2. (Color online) Execution time for high-NA BSC calculation algorithms as a function of beam NA. Our single integral calculation (labeled "Integral") is shown to be over 100 times faster than solving the appropriate linear system of equations (labeled "Inversion"). For reference, execution times are also shown for force calculation and for a two-sphere multiple scattering calculation. The timings are independent of particle size.

the force calculation. For a multisphere calculation, the speed of the BSC calculation is the limiting factor when it takes longer than the multiple scattering calculation.

Figure 1 shows the execution times for each algorithm. It also shows the time required to calculate the force on a single particle and the time required per sphere to calculate the net scattering for a group of particles, which are the other main steps in a Mie scattering calculation. Our analytical result for Bessel beams can be evaluated faster than the force on a sphere can be calculated, so the BSC calculation no longer limits the speed of the calculation. Our single-integral result for a low-NA beam ($w_0=8\lambda$) is still slower to evaluate than the force calculation, but is significantly faster than the double-integral alternative, and will not limit the speed of a two-sphere multiple scattering calculation.

For particles away from the origin, the execution time for Nieminen's approach grows very rapidly, while our integral method requires only a slightly longer execution time. For this reason, as discussed earlier, a common approach for high-NA beams is to calculate the field at the origin and then use the translation addition theorem to determine the field at other points. Hence in this case it is a fairer comparison to plot the execution time as a function of NA (see Fig. 2) instead of position or particle size.

Here too we see that our single-integral method is several hundred times faster than the technique of Nieminen *et al.* [10] using LU decomposition to solve the system of linear equations. As a result, the BSC calculation is faster than the force calculation even for a single particle, whereas solving the system of linear equations is the slowest part even of a two-sphere calculation.

5. CONCLUSION

We have presented improved expressions for calculating the beam shape coefficients (BSCs) for Bessel and Gaussian beams, for use in Mie scattering calculations. Our analytical result for Bessel beams allows the BSCs to be calculated several orders of magnitude faster than published results requiring numerical evaluation of integrals, resulting in faster Mie scattering calculations.

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